Photovoltaic effect in quantum adiabatic transport as a way to pump electrons

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We study the photovoltaic effect due to gate-voltage modulations in an asymmetric constriction. Taking a simple system as an example, we show that, under certain conditions, an integer amount of electrons per absorbed photon or per cycle can be transmitted. The interaction with the modulation occurs mainly in some resonant points along the constriction.

With the help of modern semiconductor heterostructure fabrication techniques, low-dimensional nanostructure devices can be realized, that consist of a two-dimensional electron gas (2DEG) in which an electrostatically induced geometry is defined. The electron transport through such a device shows a wealth of interesting phenomena, reflecting its quantum coherent nature.[1] This is due to the fact that the typical lengths of these geometries are of the order of the Fermi wavelength λ_F, whereas the inelastic length l_ϕ in pure materials can exceed λ_F by several orders of magnitude. Lateral confinement on a small length scale induces one-dimensional transport channels (subbands). Scattering between transport channels is almost completely suppressed, if the geometry is slowly varying in the transport direction. We then enter the regime of quantum adiabatic transport.[2] Each transport channel (with index n) is described by an effective one-dimensional potential $U_n(x)$. The electron motion can be treated in a semiclassical approximation. Depending on the position of the Fermi energy with respect to the maximum of U_n along the device, the channel is closed or open. If it is open, it contributes to the conductance the unit e^2/h. A well-known manifestation of these principles is the conductance quantization in a narrow constriction.[3]

The device itself is connected to electron reservoirs[4] by perfectly conducting leads. The reservoirs act as source and sink for electrons. At zero temperature, electrons with energies up to the Fermi level are injected into the leads. Usually, electron transport is achieved by applying a bias voltage, i.e., by keeping the electron reservoirs at a different chemical potential. However, it has been shown that transport can also be obtained with the help of a time-dependent gate-voltage or a time-dependent magnetic flux.[5–8] It turns out that a controllable electron current of the order of one electron per cycle or per flux quantum can be realized without an applied bias voltage in these so-called electron pumps.

In this paper we consider a single, asymmetric constriction, to which a gate-voltage modulation is applied. We discuss the possibility for this system to show the *photovoltaic effect.* This effect occurs, e.g., in a homogeneous bulk solid[9] and in small metallic constrictions,[10] as the appearance of a direct current under uniform illumination. A necessary condition for this effect is the absence of a spatial symmetry, leading to an asymmetry of the elementary electronic processes. A device like the photodiode, for instance, is based on the same principle.

In the case of a modulated constriction, inelastic absorption and emission may induce intersubband scattering and hence destroy adiabaticity. This scattering takes place mainly in resonance points, where the level spacing between the subbands involved equals the modulation frequency ω and the velocities in both subbands are equal.[11] If there is no mirror symmetry with respect to a plane perpendicular to the transport direction of the constriction, these electronic processes are noninvariant under spatial inversion within the one-dimensional transport channels. As a result, they predominantly occur in one particular resonant point, and a frequency-dependent net current of the order of a few electrons per cycle can be realized without an applied bias voltage.

A time-dependent modulation in general can give rise to a wealth of inelastic and elastic transitions, leading to a variety of transport phenomena. Without going into details, we will focus on the possibility of controllable electron transport in the system considered above. We will present the conditions under which a fixed amount of electrons transmitted per cycle and per absorbed photon can be realized.

Consider the geometry depicted in Fig. 1. In the adiabatic limit $d/R \ll 1$,[2] where d is the local width of the constriction and R the local radius of curvature, the nth transport channel is described by the effective potential $U_n(x)$, shown in Fig. 2. If all the open transport channels are transmitted with unity probability, the adiabatic wave function at energy E in subband n can be written in the WKB approximation as

$$\Psi_{nE}(x)=e^{iS_{nE}(x)} \tag{1}$$

with the classical action

$$S_{nE}(x)=\int_{-\infty}^{x} dx' k_{nE}(x') ,$$

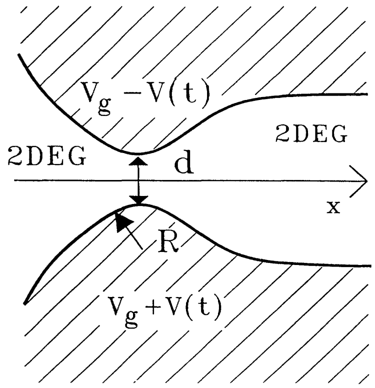

FIG. 1. 2DEG with an asymmetric constriction, characterized by a local width d and a local radius of curvature R. To the gate dc voltage V_g a small additional modulation $V(t)$ can be added. The gates are modulated with a relative phase shift of π, such that the constriction is only shifted.

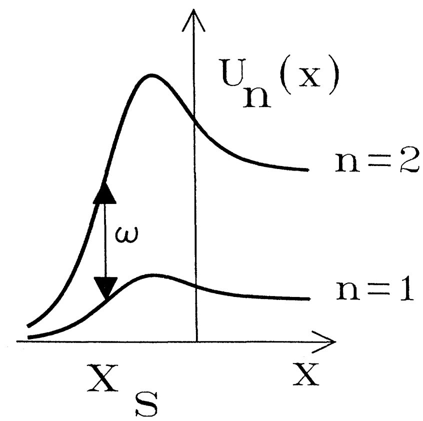

FIG. 2. Set of independent one-dimensional effective potentials $U_n(x)$ as a function of x for the asymmetric constriction of Fig. 1. The asymmetry gives rise to a different subband splitting ΔE_{sub} right and left to the maximum. One saddle point is situated at x_s.

defined with the help of the local momentum

$$k_{nE}(x')=\sqrt{2m\,[E-U_n(x)]}\ .$$

The adiabatic limit is valid on the adiabatic length $\sqrt{dR}$; outside this region, geometrically induced mixing of transport channels becomes important.

We consider a gate-voltage modulation which shifts the constriction by an amount δd, without changing the width d. This can be obtained by applying a modulation to both gates of opposite sign. The effect of this is described by a time-dependent matrix element[11]

$$\Lambda_{nn'}(x)\cos(\omega t)\ . \tag{2}$$

This matrix element accounts for possible scattering processes from channel n' into n. If the lateral confinement of the constriction is modeled as an infinite square well, we have

$$\Lambda_{nn'}(x)=-2\frac{nn'\pi^2\,\delta d}{md^3}\equiv-4nn'E_g(x)\frac{\delta d}{d} \tag{3}$$

which is valid if $\delta d/d \ll 1$. The ground-state energy in the well is $E_g(x)$, m is the effective mass of the electron. Since the perturbation merely shifts the constriction periodically back and forth, the only allowed transitions are *intersubband* processes between even and odd states in the constriction. No *intrasubband* processes $(n=n')$ will occur.

It is instructive to study the effect of the time-dependent matrix element (2) perturbatively in first order.[11] The solution of the time-dependent Schrödinger equation is written as

$$\Psi_n(x,t)=e^{-iEt}a_n(x,t)\Psi_{nE}(x)\ .$$

In first order, the amplitude $a_n(x,t)$ then satisfies the semiclassical equation

$$i\frac{\partial}{\partial t}a_n^{(1)}(x,t)=-\frac{i}{2}\left[\frac{k_{nE}(x)}{m}\frac{\partial}{\partial x}+\frac{\partial}{\partial x}\frac{k_{nE}(x)}{m}\right]a_n^{(1)}(x,t)+\Lambda_{ni}(x)\cos(\omega t)\frac{\Psi_{iE}(x)}{\Psi_{nE}(x)}\ . \tag{4}$$

Its solution reads

$$a_n^{(1)}(x,t)=A_{ni}^{(1)}(x,\omega)e^{i\omega t}+A_{ni}^{(1)}(x,-\omega)e^{-\omega t}\ , \tag{5}$$

where

$$A_{ni}^{(1)}(x,\omega)=-i\frac{m}{2}e^{-i\omega\tau_{nE}(x)}\int_{-\infty}^{x}dx'\exp\left[i\int_{-\infty}^{x'}dx''[k_{iE}(x'')-k_{nE-\omega}(x'')]\right]\frac{\Lambda_{ni}(x')}{k_{nE}(x')} \tag{6}$$

and the traversal time

$$\tau_{nE}(x)=\int_{-\infty}^{x}dx'\frac{m}{k_{nE}(x')}\ .$$

This describes inelastic scattering from an incoming transport channel i into an outgoing channel n by an inelastic first-order process involving a quantum ω. The probability for intersubband scattering can be obtained by performing the integral over x' in Eq. (6) in a saddle-point approximation. The saddle-point condition reads $k_{iE}(x_s)-k_{nE-\omega}(x_s)=0$. This means that the main contribution for scattering from subband i into n originates from the point x_s, where the velocities in both subbands are equal. The matrix element (3) at the saddle point is given by $\Lambda_{ni}(x_s)=-4\omega(ni/|n^2-i^2|)(\delta d/d)$. We find

$$|A_{ni}^{(1)}(\infty,\omega)|^2 \propto \left[\frac{ni}{|n^2-i^2|}\right]^2 \omega\tau_{\rm trav}\left[\frac{\delta d}{d}\right]^2 , \quad (7)$$

where $\tau_{\rm trav}$ is the time needed to cross the constriction. We will go beyond perturbation theory in the applied modulation by taking the neighborhood of the saddle point into account via a linearization around x_s.

The asymmetric constriction in Fig. 1 can be characterized by the fact that the typical subband splitting right and left to the constriction is different: $\Delta E_{{\rm sub},r}\neq\Delta E_{{\rm sub},l}$. We operate at frequencies $\Delta E_{{\rm sub},l}\simeq\omega<\Delta E_{{\rm sub},r}$, such that the inelastic intersubband transitions occur only left to the constriction. In the remaining part of this paper we assume that the scattering occurs only between the two lowest subbands $n=1,2$. All the other subbands are completely closed. The time-dependent Schrödinger equation can be written as the coupled set:

$$\begin{aligned} i\frac{\partial}{\partial t}\Psi_1(x,t) &= \left[\frac{-1}{2m}\frac{\partial^2}{\partial x^2}+U_1(x)\right]\Psi_1(x,t) \\ &\quad +\Lambda_{12}(x)\cos(\omega t)\Psi_2(x,t) , \\ i\frac{\partial}{\partial t}\Psi_2(x,t) &= \left[\frac{-1}{2m}\frac{\partial^2}{\partial x^2}+U_2(x)\right]\Psi_2(x,t) \\ &\quad +\Lambda_{21}(x)\cos(\omega t)\Psi_1(x,t) , \end{aligned} \quad (8)$$

which we solve by a wave function of the form

$$\begin{aligned} \Psi_1(x,t) &= e^{-iEt}a_1(x) \\ &\quad \times\exp\left[\frac{i}{2}\int_{-\infty}^{x}dx'[k_{1E}(x')+k_{2E+\omega}(x')]\right] , \\ \Psi_2(x,t) &= e^{-i(E+\omega)t}a_2(x) \\ &\quad \times\exp\left[\frac{i}{2}\int_{-\infty}^{x}dx'[k_{1E}(x')+k_{2E+\omega}(x')]\right] . \end{aligned} \quad (9)$$

These wave functions are taken at different energies E and $E+\omega$, to allow for inelastic transitions between them. Substituting (9) into (8), using the semiclassical approximation and linearizing around the saddle point x_s we find

$$\begin{aligned} 2ik_s\frac{d}{dy}a_1(y) &= -\beta_s y a_1(y)+m\Lambda_{12}(x_s)a_2(y) , \\ 2ik_s\frac{d}{dy}a_2(y) &= \beta_s y a_2(y)+m\Lambda_{21}(x_s)a_1(y) , \end{aligned} \quad (10)$$

where $y=x-x_s$, k_s is the momentum at the saddle point and $\beta_s=m\omega/\sqrt{dR}$. This equation describes a level-crossing problem, as one encounters, e.g., in the context of Zener tunneling.[12] By studying the asymptotic behavior of the solution a_1 and a_2, we find the transition probabilities P_{12} and P_{21} for intersubband processes under absorption and emission, respectively, of a quantum ω:

$$P_{12}(\omega)=P_{21}(\omega)\equiv P(\omega)=1e^{-\pi a_s} \quad (11)$$

with $a_s=m^2\Lambda^2(x_s)/2k_s\beta_s$. Note that a first-order expansion in Λ^2 yields the result (7). The fact that $P_{12}=P_{21}$ is due to the fact that the Hamiltonian is invariant under time reversal.

We can calculate the current through the constriction by subtracting the current from right to left I_{rl} from the corresponding current I_{lr}, taking[11]

$$I_{lr}=\frac{e}{\pi}\int dE\int dE' f_l(E)[1-f_r(E')]T_{ni}^{rl}(E',E) . \quad (12)$$

The current which flows through the constriction is characterized by a scattering probability $T_{ni}^{rl}(E',E)$ for a particle with energy E in subband i, transmitted from left to right into subband n with energy E'. The Fermi factors f_r and f_l indicate the reservoirs, right and left to the constriction, respectively, that are in thermal equilibrium. Due to time reversibility, the scattering probabilities satisfy

$$T_{ni}^{rl}(E',E)=T_{in}^{lr}(E,E')$$

and the total current reads

$$I=\frac{e}{\pi}\int dE\int dE'[f_l(E)-f_r(E')]T_{ni}^{rl}(E',E) . \quad (13)$$

Suppose the lowest subband is completely transmitted, whereas the second subband is closed. Neglecting the dependence of $P(\omega)$ on E, we perform the integration over energy in Eq. (13). We find the total current, pumped through the constriction by the modulation

$$\begin{aligned} I &= -\frac{e}{\pi}\omega P(\omega) \\ &= -\frac{e}{\pi}\omega\left\{1-\exp\left[-\tfrac{32}{9}\pi\omega\tau_{\rm trav}\left[\frac{\delta d}{d}\right]^2\right]\right\} . \end{aligned} \quad (14)$$

It is worthwhile to emphasize that the exponent in (14) can be made arbitrarily small. If $\omega\gg 1/\tau_{\rm trav}$, which may well be the case, only slight shifts, $\delta d/d\ll 1$, cause the probability $P(\omega)$ to be almost unity. If $P(\omega)=1$, the current is

$$I=-\frac{e}{\pi}\omega=-2e/T , \quad (15)$$

where T is the period of the modulation. The fact that two electrons are transmitted per cycle is due to the twofold spin degeneracy of the subband. The net electron-current flows from right to left, since the resonant point is situated left to the constriction. When a photon is absorbed in this resonant point, it produces an electron-hole pair. There are two possibilities: (i) the electron moves from left to right in the second subband and the hole from right to left in the first subband or (ii) the electron moves from right to left in the second subband and the hole from left to right in the first subband. If both subbands are open, these processes compensate one another. If the upper subband is closed, the electron in process (i) is reflected at the constriction and does not contribute to the current. As a result, one electron per two absorbed photons is transmitted from right to left in this case. The importance of the asymmetry is clear from the discussion above: a second saddle point right to the constriction would provide an opportunity for electrons, transmitted from left to right to compensate the effect. In general we always expect a net current if the Hamiltonian is noninvariant under the transformation $x \rightarrow -x$.

In a real experiment, both intersubband and intrasubband processes will occur, since perfect parity for lateral confinement will not be realized. However, at frequencies exceeding $1/\tau_{\mathrm{trav}}$ in an adiabatic constriction, the probability for intrasubband processes is exponentially small. Another complication will be that transitions between subbands with higher indices $n > 2$ will occur. As long as only the lowest subband is transmitted, these transitions will not change the effect qualitatively. In a typical constriction,[3] the subband splitting is about 1.3 meV, leading to frequencies needed to see the photovoltaic effect that are of the order of 10^{12} Hz. We can scale down these frequencies by increasing the system size.

In conclusion we discussed the possibility of finding the photovoltaic effect in a modulated constriction without mirror symmetry. If the modulation only shifts the constriction back and forth without changing its width, inelastic intrasubband processes are induced at resonant points near the constriction. Due to the asymmetry of the constriction the transitions preferably occur in one of these resonant points, resulting in a controllable net current through the device, which is two electrons per cycle under appropriate limiting conditions.

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